Monte Carlo generators for top quark production in the LHC

15th International Workshop on Top Quark Physics

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on behalf of the CMS and ATLAS Collaborations

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Introduction

- MC simulation is a crucial ingredient in top quark analyses:
  - good modelling of data and high accuracy predictions for interpretations
  - uncertainties are a limiting factor in many precision measurements and searches
- ATLAS and CMS use same generators but have different modelling uncertainty prescriptions:
  - understanding how to combine the differing strategies of ATLAS and CMS is critical
  - ➩ LHCtopWG is ideal forum to discuss how to reduce modelling systematics

Outline

- Interpretation of the MC top mass parameter in ATLAS MC (ATL-PHYS-PUB-2021-034)
- ATLAS studies of the interference tt/tW (ATL-PHYS-PUB-2021-042)
- ATLAS studies of ttbb and ttW (ATL-PHYS-PUB-2022-026)
- CMS PYTHIA 8 colour reconnection tunes based on underlying-event data (CMS-GEN-17-002)
- CMS and ATLAS common top MC sample (ATLAS-PHYS-PUB-2021-016, CMS-NOTE-2012-05)

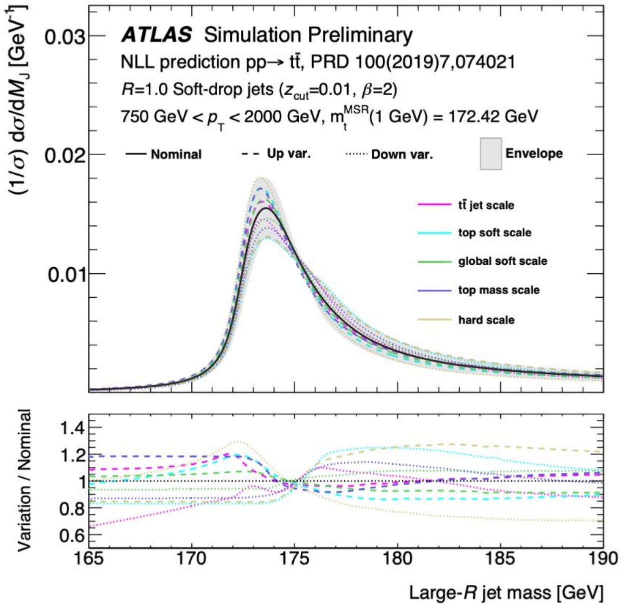
Interpretation of the top mass parameter in ATLAS MC

ATL-PHYS-PUB-2021-034

- Can the top mass parameter in ATLAS MC samples be identified with a well-defined mass scheme below 500 MeV?
- Study the interpretation in light of a renormalized mass in the MSR scheme (Phys. Rev. Lett. **101**, 151602)
  - With the scale R set to 1 GeV is numerically close to the pole mass (R=0 GeV)

$$m_{top}^{MC} = m_{top}^{MSR}(R) + \Delta m^{MSR}$$

- A calibration is performed by comparing ATLAS MC predictions to a calculation at next-to-leading-logarithm (NLL) accuracy
  - Two models: Powheg + Pythia 8 or Herwig 7 ($m_{top,MC}$ is set to 172.5 GeV)
  - Differential jet mass cross section at particle level
    - Strong sensitivity to m_{top} in the jet mass peak ➪
  - Main ingredients:
    - Inclusive treatment of hadronic top quark decays
    - Light soft-drop grooming to remove soft-wide radiation
    - Three free parameters: m_{top}, and $\Omega_{1q}^{\circledcirc}$ and x_2 to account for non-perturbative hadronization effects
    - Does not account for underlying event (UE) effects
      - MC templates of Var1 variations of A14 tune and alternative colour reconnection (CR) models used to estimate impact on mass



Interpretation of the top mass parameter in ATLAS MC

ATL-PHYS-PUB-2021-034

- Use a chi-square fit to find the prediction that best describes MC
  - With Powheg+Pythia 8

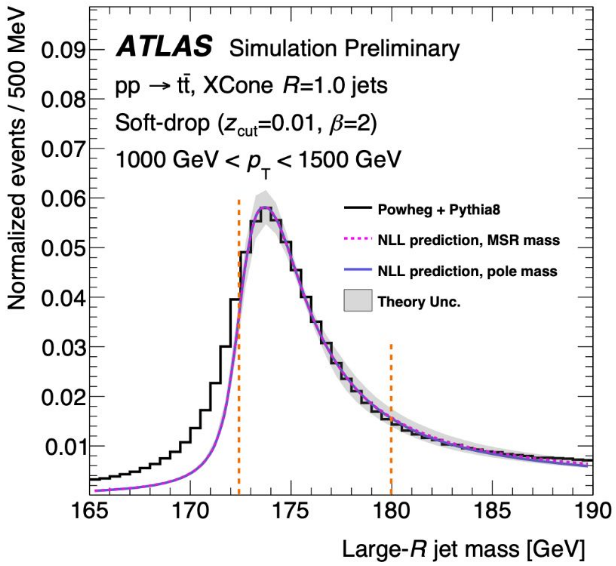
$$\boxed{m_{top}^{MSR}(1\ GeV) = 172.42 \pm 0.10\ (stat.)\ GeV}$$

$$\Downarrow$$

$$\boxed{m_{top}^{MC} = m_{top}^{MSR}(1\ GeV) + 80^{+350}_{-410}\ MeV}$$

  - Theoretical uncertainties dominate

Source	Size [MeV]	Comment
Theory (higher-order corrections)	+230/−310	Envelope of NLL scale variations
Fit methodology	±190	Choice of fit range, p_T bins
Underlying Event model	±155	A14 eigentune variations, CR models
Total Systematic	**+340/−340**	
Statistical Uncertainty	±100	
Total Uncertainty	**+350/−410**	

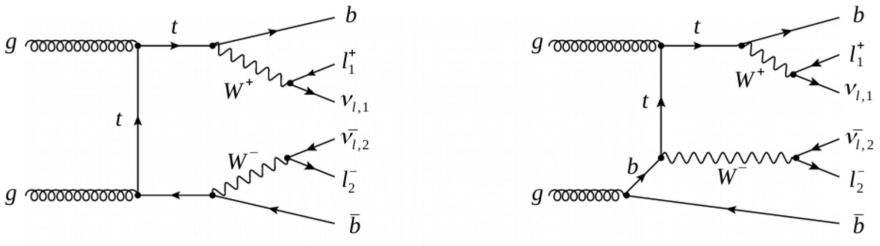


  - Similar results with Powheg and Herwig 7 even if both models predict very different jet mass distributions
  - MSR-MC mass relation found to be stable within 200 MeV with the restrictions imposed by the theory
  - Future advances in the formal accuracy of the theory calculation and in the treatment of non-perturbative corrections may lead to a sizeable reduction of the systematic uncertainties (Phys. Rev. Lett. 117, 232001)
  - This relation works best with a direct mass measurement with boosted top quarks and the same observable

Study of the interference tt/tW in bbll$\nu\nu$ events in ATLAS

ATL-PHYS-PUB-2021-042

- Handling of interference between tt production and tW long-standing issue
  - separate samples for tt and tW so far used in ATLAS



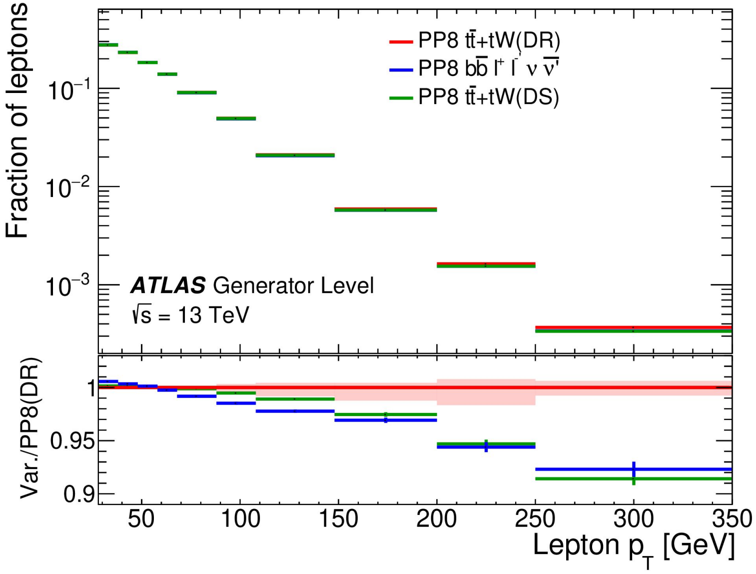
- Overlap treated via diagram-removal (DR) or diagram-subtraction techniques (DS) applied on tW samples *(Eur.Phys.J.C(2017))*
  - DR: remove diagrams that also enter tt pair production
  - DS: subtract resonant tt contributions locally introducing a gauge invariant subtraction term

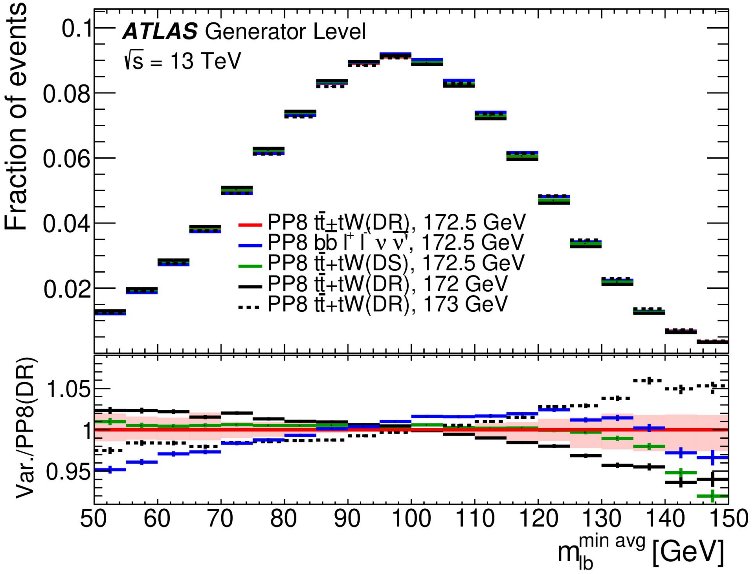
- New bb4l generator includes theoretical improvements in the simulation of tt processes (*Eur. Phys. J. C* 76, 691 (2016))
  - Next-to-leading order (NLO) matrix element (ME) generator for pp→bbl+lνν implemented in Powheg
  - includes tt-tW interference effects, off-shell effects, and top decays at NLO
- Events from bb4l interfaced to Pythia 8 for the parton shower in this study

Study of the interference tt/tW in bbll$\nu\nu$ events in ATLAS

ATL-PHYS-PUB-2021-042

- The studies are performed in a phase-space for typical *tt* precision measurements and in phase-spaces relevant for searches.



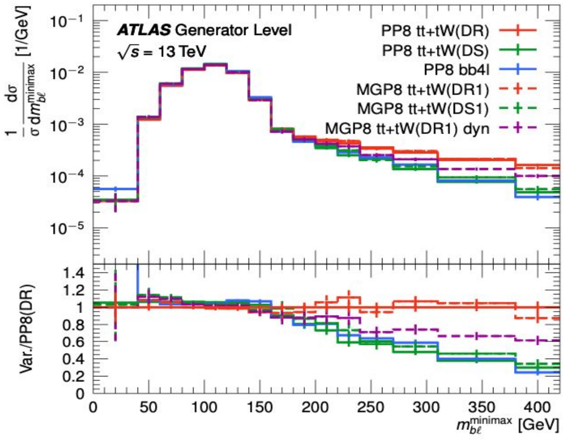


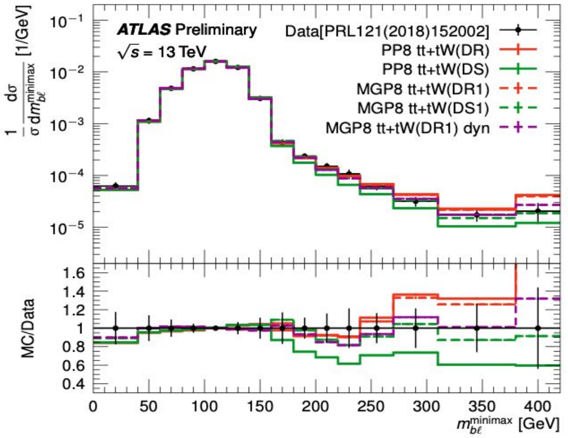
⇨ Better agreement of DS in some distributions like the lepton p_T and the $m_{\ell b}^{\mathrm{minavg}}$ variable

Study of the interference tt/tW in bbll$\nu\nu$ events in ATLAS

ATL-PHYS-PUB-2021-042

- Different DS and DR scheme implemented in MadGraph5_aMC@NLO compared to data in a search-like phase space with large missing energy and to bb4l predictions
- Predictions using the DR scheme agree well between Powheg and MG
- The DS scheme shows significant differences in $m_{\ell b}^{\mathrm{minavg}}$
- The differences are not visible in the SUSY search region
- Studies show that DR with a dynamical scale and the DS scheme have a better agreement with the *bb*4l setup than the nominal DR scheme.
- Current systematic prescription based a comparison of the DR vs. DS scheme
  - suggest to use the DR scheme with a dynamic scale instead of the sample with a fixed scale.



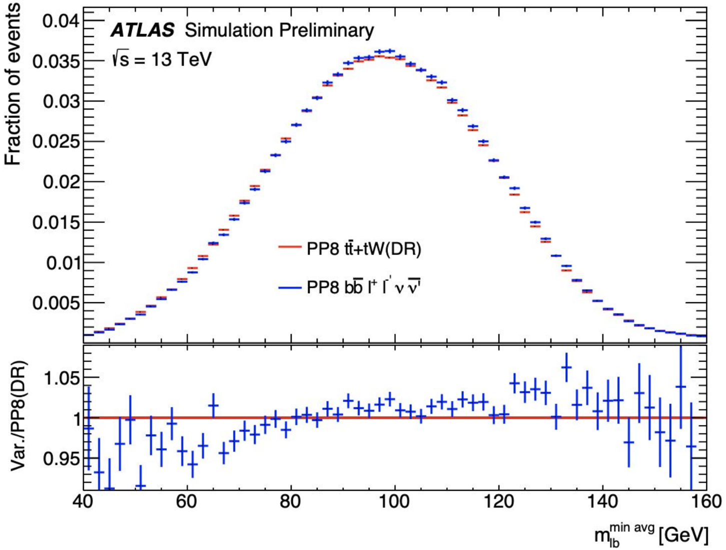


Study of the interference tt/tW in bbll$\nu\nu$ events in ATLAS

ATL-PHYS-PUB-2021-042

- ATLAS measurements of m_{top} based on template fit use tt and tW events simulated with the hvq generator of Powheg

- Impact of bb4l estimated using strategy from 8TeV measurement
  - using tt and tW hvq Powheg+Pythia 8 samples as templates
  - unbinned likelihood fit to the $m_{\ell b}^{\mathrm{minavg}}$ observable
  - find value of m_{top} that best describes bb4l prediction



- bb4l gives a shift of the top mass of 0.36 ± 0.08 GeV of a similar size as the total signal modelling uncertainty of 0.35 GeV in the current ATLAS result in Phys. Lett. B **761** (2016) 350

Study of ttbb and ttW for ttH analyses in ATLAS

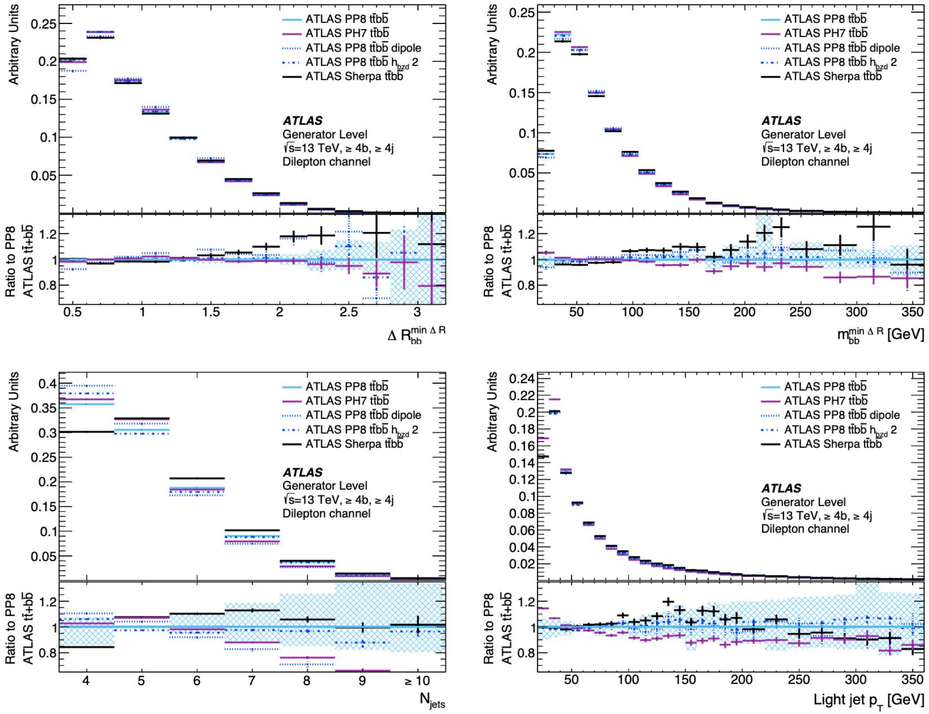
ATL-PHYS-PUB-2022-026

- *ttbb* and *ttW* modelling is a limiting factor in *ttH* (*H-> bb* or multi-lepton)

- Two sets of generator predictions used by ATLAS in a typical phase space of the *ttH*(*H* → *bb*) measurement:
    - the generators used in the most recent published analyses involving *tt* inclusive predictions based on 5FS scheme to estimate uncertainties
    - new ttbb systematic model based on ttbb@NLO ME on 4FS

- The difference between both predictions exceeds the uncertainties from the scale variations

- New ttbb systematic model shows reduced sensitivity to parton shower variations and to NLO generator

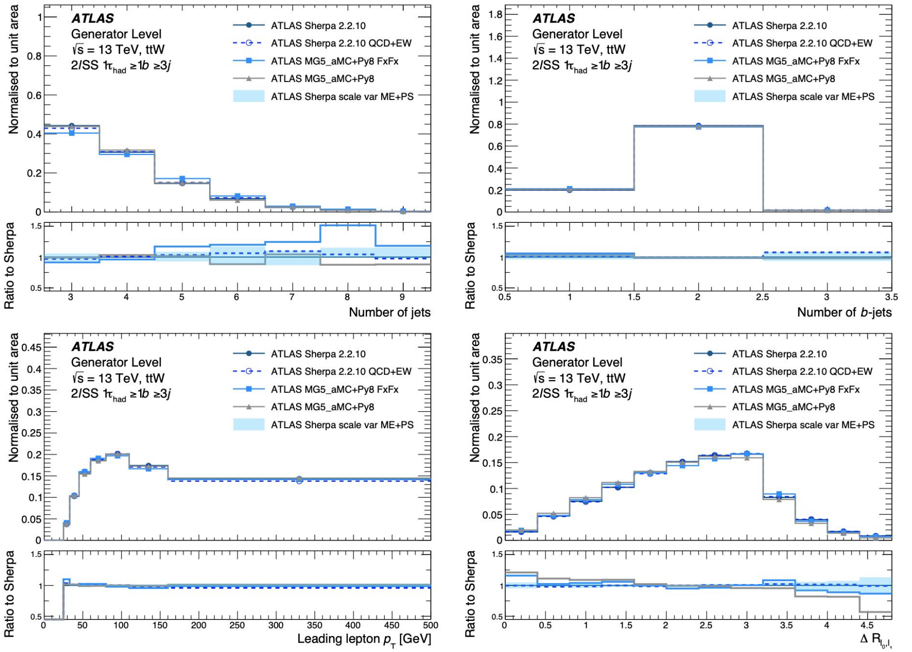


* PDF in 4 flavour scheme (FS) does not contain b quarks: all b quarks generated in ME and cannot directly come from the (anti)proton. In 5FS PDF contains g → bb splitting.

Study of ttbb and ttW for ttH analyses in ATLAS

ATL-PHYS-PUB-2022-026

- Compared *ttW* predictions of Sherpa and MG5_aMC@NLO+Pythia8 in regions and observables relevant for the measurement of *ttH* multi-lepton
- Overall, the differences between the different model predictions are mostly within the scale uncertainty band except at the edges of the phase space.
- Inclusion of electroweak (EW) effects only cause minor shape effects but lead to higher xsec especially at high jet multiplicity.
- Inclusion of FxFx into the MG5 predictions leads to significant effects in jet based distributions, especially at low H_T and generally better agreement with Sherpa
- These distributions will be used in future comparisons with CMS



* The different jet multiplicities are merged using the FxFx NLO matrix-element and parton-shower merging prescription (*J. High Energ. Phys.* 2012, 61 (2012))

Pythia 8 color reconnection tunes based on UE data in CMS

CMS-GEN-17-002

- Both CMS and ATLAS have a set of standard recommendations to assess uncertainties in top-quark-related analyses
  - Matrix-elements scale variations
  - PDF4LHC recommendations
  - Top quark p_T modelling and mass are very analysis-dependent
- Uncertainties on the parton shower generator

Systematic unc.	CMS	ATLAS
ISR and FSR	Independent μ_R^{ISR} , μ_R^{FSR} scale variations with factor (2,0.5)	
UE	Variation of CP5 / A14 tune	
CR	Retuning UE with different CR models	
b fragmentation	Variations of Bowler-Lund r_B parameter of fragm. function	
Fragmentation & hadronization	Pythia 6 vs Herwig++ impact on jet energy response	Pythia 8 vs Herwig 7
Hadron decays	Varying B semi-leptonic BF within PDG value uncertainties	
Generator / NLO matching scheme	Powheg vs MC@NLO as cross-check	Powheg vs MC@NLO as uncertainty
ME-PS matching	Variation of h_{damp} that regulates first high-p_T emission	

⇦ Eur. Phys. J. C 80 (2020) 4, JHEP 03 (2017) 157

⇦ ATL-PHYS-PUB-2017-008,**NEW: CMS-GEN-17-002**

⇦ CMS-PAS-TOP-18-012, ATLAS-CONF-2020-050

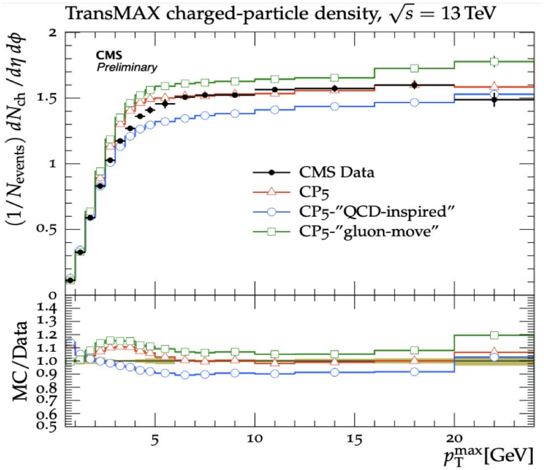
⇦ JHEP 02 (2019) 149, ATL-PHYS-PUB-2020-023

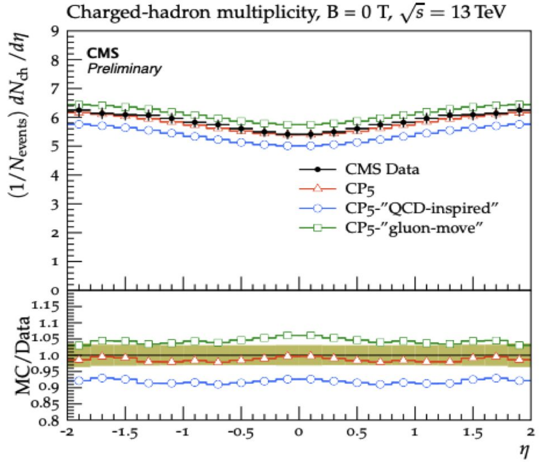
⇦ CMS-PAS-TOP-16-021, ATL-PHYS-PUB-2020-023

Pythia 8 color reconnection tunes based on UE data in CMS

CMS-GEN-17-002

- Color reconnection uncertainties on the parton shower typically evaluated re-tuning the UE with different CR models
- This study includes additional models implemented in Pythia 8
  - MPI-based (default CP5)
  - **QCD-inspired** (CP5-CR1). Adds the QCD colour rules on top of the minimisation of the string length
  - **Gluon-move** (CP5-CR2). Moves the final-state gluons to a string piece belonging to different colour connected partons
- Tune obtained by constraining simultaneously the parameters controlling the contributions of the multiparton interactions (MPI) and of the CR model
- New tunes achieve a very good level of agreement against many UE observables including UE data measured at forward pseudo-rapidities.
- Models after tuning perform no better than the CP5 tune for the observables presented in this study.
- Unfortunately, this still does not reduce uncertainty in top mass measurement

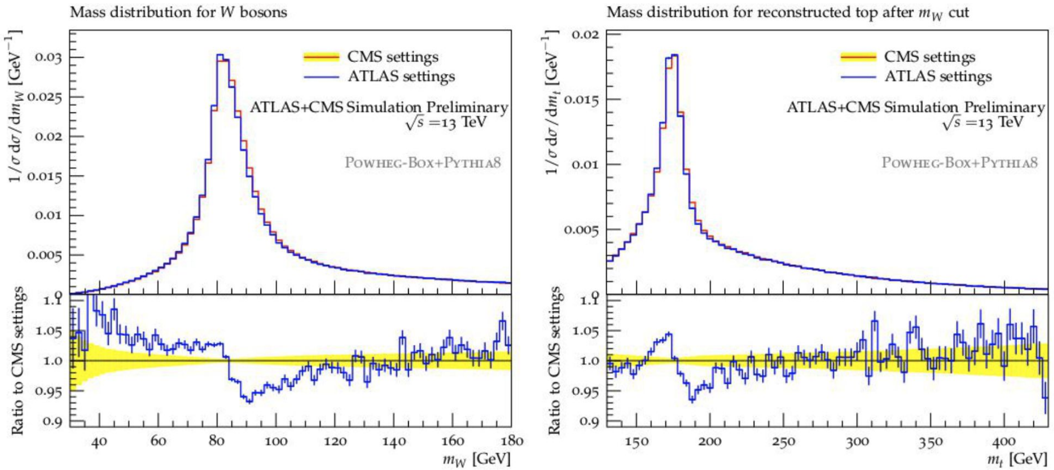




Towards common $t\bar{t}$ MC settings for ATLAS and CMS

ATL-PHYS-PUB-2021-016, CMS-NOTE-2021-005

- ATLAS and CMS use the same generators to model the tt process, but different settings and uncertainty prescriptions, making combinations challenging.



Source: LHCtopWG

- A tt sample with common settings would facilitate combinations and comparisons
  - Help to understand correlations of systematic uncertainties due to MC modelling
  - Easier to understand the trends in similar analyses with slightly different selections or binnings
  - Share the computing resources
- Effort carried out in the LHCtopWG
  - Mike Fenton (ATLAS), Dominic Hirschbuehl (ATLAS), Reinhard Schwienhorst (ATLAS) and Giulia Negro (CMS)

Towards common $t\bar{t}$ MC settings for ATLAS and CMS

ATL-PHYS-PUB-2021-016, CMS-NOTE-2021-005

- ATLAS and CMS use Powheg+Pythia8 MC simulations to model the tt process, but different configurations
- Many parameters are different: Powheg revision & settings, Pythia8 version & settings, usage of EvtGen, etc.

Setting name	Setting description	CMS default	ATLAS default	Common Proposal
Powheg				
qmass	top-quark mass [GeV]	172.5	172.5	172.5
twidth	top-quark width [GeV]	1.31	1.32	1.315
hdamp	first emission damping parameter [GeV]	237.8775	258.75	250
wmass	$W^\pm$ mass [GeV]	80.4	80.3999	80.4
wwidth	$W^\pm$ width [GeV]	2.141	2.085	2.11
bmass	b-quark mass [GeV]	4.8	4.95	4.875
Pythia 8				
	Pythia 8 version	v240	v230	v240 (CMS) v244 (ATLAS)
	Tune	CP5	A14	Monash
PDF:pSet	LHAPDF6 parton densities to be used for proton beams	NNPDF31_nnlo _as_0118	NNPDF23_lo _as_0130_qed	NNPDF23_lo _as_0130_qed
TimeShower:alphaSvalue	Value of α_s at Z mass scale for Final State Radiation	0.118	0.127	0.1365
SpaceShower:alphaSvalue	Value of α_s at Z mass scale for Initial State Radiation	0.118	0.127	0.1365
MPI:alphaSvalue	Value of α_s at Z mass scale for Multi-Parton Interaction	0.118	0.126	0.130
MPI:pT0ref	Reference p_T scale for regularizing soft QCD emissions	1.41	2.09	2.28
ColourReconnection:range	Parameter controlling colour reconnection probability	5.176	1.71	1.80

- Common Settings (version 0.1) are for a setup of Powheg+Pythia8, the Monash Pythia8 tune, NNPDF2.3 LO PDF set, and approximately average values for the various physical and technical settings that are different between experiments

Towards common $t\bar{t}$ MC settings for ATLAS and CMS

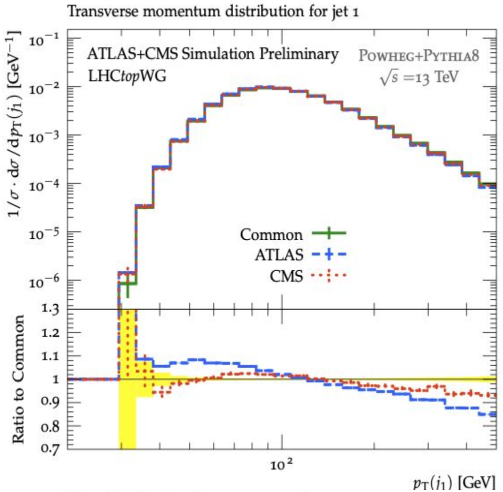
[ATL-PHYS-PUB-2021-016](), [CMS-NOTE-2021-005]()

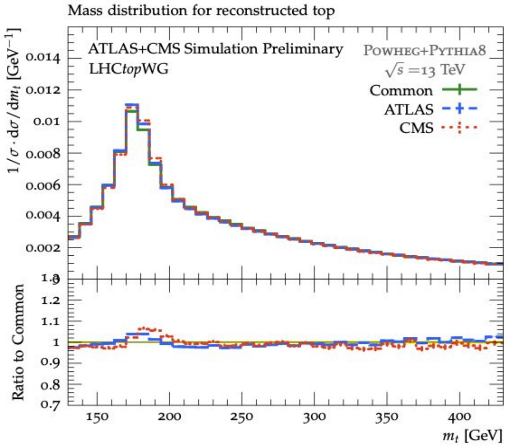
Common settings vs ATLAS and CMS nominal settings

- Good agreement is observed between all three samples in angular distributions sensitive to spin correlation effects
- Disagreement found in many distributions, particularly those related to jet kinematics and resonance masses
- Both the W mass and the top mass are shifted slightly in the peak of the distribution for the common sample
- Both the m_{tt} and m_{lb} distributions show overall good agreement

Next steps

- Sample v0.2 with more “physical” settings ready
- Comparison to ATLAS & CMS nominal samples and data
- Additional RIVET routines
- Preliminary note draft being finalized





Summary and conclusions

- First interpretation of the MC top-quark mass parameter in the MSR scheme at 1 GeV in ATLAS
    - Improvement in the accuracy of the theory calculation and in the treatment of UE may lead to a sizeable reduction of the systematic uncertainties
- ATLAS studies of the interference tt/tW
    - The bb4l generator provides a better description of the tt/tW interference and off-shell effects than current generators
    - DS or DR with dynamical approach better agreement with bb4l prediction that DR
    - Impact on m_{top} within modelling uncertainties of current ATLAS measurement
- First tests with new ttbb systematic model
    - Reduced sensitivity to parton shower variations and to NLO generator
- Different model predictions of ttW are mostly within the scale uncertainty band
- New CMS PYTHIA 8 colour reconnection tunes based on underlying-event data
    - Includes new CR models. Still does not reduce uncertainty in most precise mass measurement
- CMS and ATLAS common top MC sample
    - Common sample v0.1 settings (not yet optimized to data) and comparisons public
    - ➪ Currently working on comparison of new sample v0.2 with more "physical" settings to ATLAS & CMS nominal samples and data

Thanks

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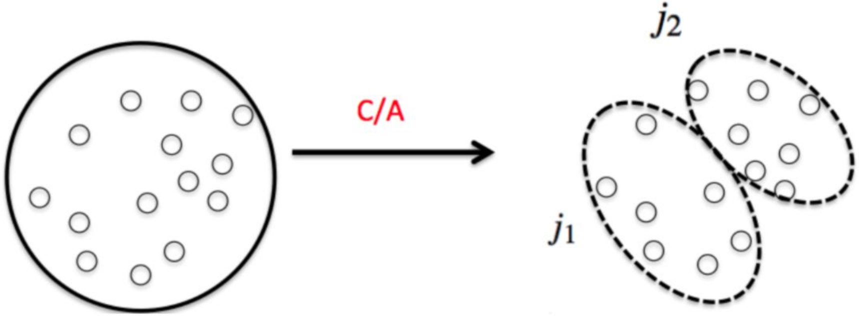
The Soft Drop algorithm

JHEP **05**, 146 (2014)

- Take a jet, re-cluster its constituents with C/A, and go backwards in the C/A clustering sequence



- If $$\frac{\min(p_{T,1}, p_{T,2})}{p_{T,1}+p_{T,2}} > z_{cut}\left(\frac{\Delta R_{12}}{R}\right)^{\beta}$$ the jet is a soft drop jet.

- Otherwise, the highest p_T sub-jet is taken as a new candidate and the procedure is iterated.

- z_{cut} sets the scale of energy removal. Higher z_{cut} means more energy removed by grooming.

- β determines the sensitivity to wide-angle radiation.
    - Larger β means smaller fraction of soft small-angle radiation removed -> less grooming.

Study of the interference tt/tW in bbll$\nu\nu$ events in ATLAS

ATL-PHYS-PUB-2021-042

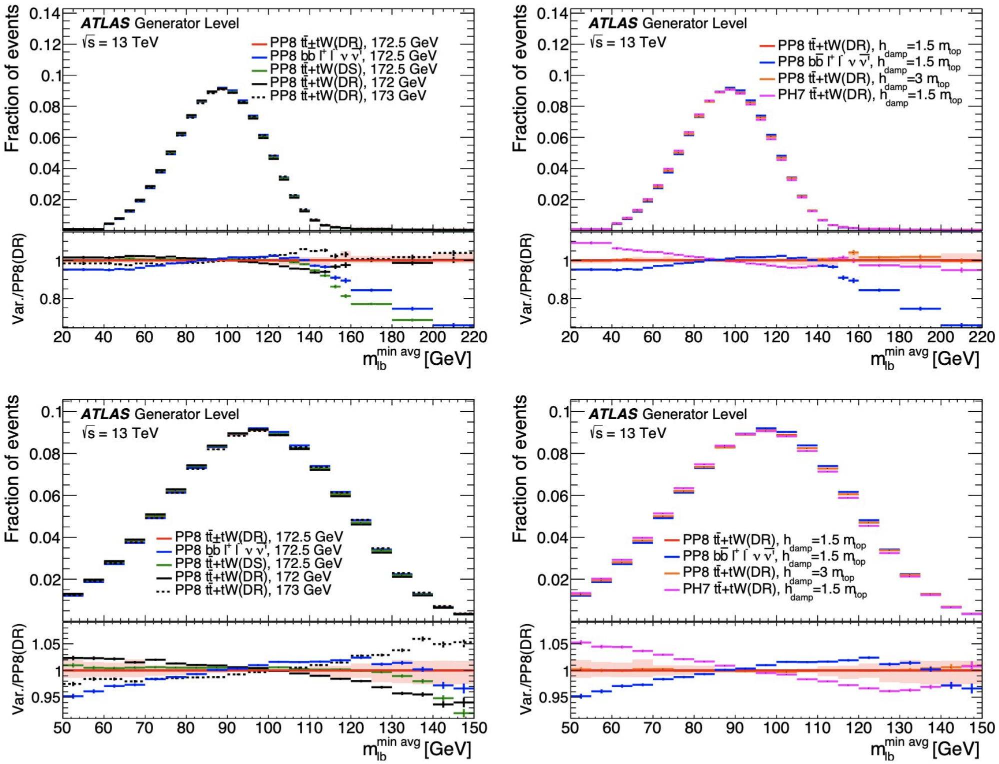
Final state	$t\bar{t}$	$bb4\ell$
Generator	hvq [10]	$bb4\ell$ [6]
Framework	POWHEG-BOX	POWHEG-BOX-RES
NLO matrix element	$t\bar{t}$	$b\bar{b}\ell^+\ell^{-'}\nu\bar{\nu}'$
Decay accuracy	LO+PS	NLO+PS
NLO radiation	single	multiple
Spin correlation	approx.	exact
Off-shell $t\bar{t}$ effects	BW smearing	exact
tW and non-resonant effect	no	exact
b-quark massive	yes	yes

Study of the interference tt/tW in bbll$\nu\nu$ events in ATLAS

ATL-PHYS-PUB-2021-042

- The invariant mass of the lepton-*b*-jet combination with the lowest average m_{lb} value

$$m_{\ell b}^{\text{minavg}} = \min\{\frac{m_{\ell_1,b_1} + m_{\ell_2,b_2}}{2}, \frac{m_{\ell_1,b_2} + m_{\ell_2,b_1}}{2}\}$$



Study of ttbb and ttW for ttH analyses in ATLAS

ATL-PHYS-PUB-2022-026

	name	ME	Generator	ME order	Shower	Tune	NNPDF PDF set	h_{damp}	h_{bzd}	$\sigma^{\geq 1\mathrm{lep}}$ [pb]
ATLAS	PP8 $t\bar{t}b\bar{b}$	$t\bar{t}b\bar{b}$	Powheg-Box-Res	NLO	Pythia 8.224	A14	4FS 3.0 NLO as 0118	$H_T/2$	5	18.72
ATLAS	PP8 $t\bar{t}b\bar{b}$ h_{bzd} 2	$t\bar{t}b\bar{b}$	Powheg-Box-Res	NLO	Pythia 8.224	A14	4FS 3.0 NLO as 0118	$H_T/2$	2	18.46
ATLAS	PP8 $t\bar{t}b\bar{b}$ dipole	$t\bar{t}b\bar{b}$	Powheg-Box-Res	NLO	Pythia 8.224	A14, dipoleRecoil	4FS 3.0 NLO as 0118	$H_T/2$	2	18.72
ATLAS	PH7 $t\bar{t}b\bar{b}$	$t\bar{t}b\bar{b}$	Powheg-Box-Res	NLO	Herwig 7.1.6	default	4FS 3.0 NLO as 0118	$H_T/2$	5	18.47
ATLAS	Sherpa $t\bar{t}b\bar{b}$	$t\bar{t}b\bar{b}$	Sherpa 2.2.10	NLO	Sherpa	default	4FS 3.0 NNLO as 0118	—	—	20.24
ATLAS	PP8 $t\bar{t}$	$t\bar{t}$	Powheg v2	NLO	Pythia 8.210	A14	5FS 3.0 NLO	$1.5 \cdot m_{\mathrm{top}}$	5	451.78
ATLAS	PH7 $t\bar{t}$	$t\bar{t}$	Powheg v2	NLO	Herwig 7.13	default	5FS 3.0 NLO	$1.5 \cdot m_{\mathrm{top}}$	5	451.78[c]
ATLAS	aMC+P8 $t\bar{t}$	$t\bar{t}$	MG5_aMC@NLO	NLO	Pythia 8.210	A14	5FS 3.0 NLO	—	—	451.78[c]

Study of ttbb and ttW for ttH analyses in ATLAS

ATL-PHYS-PUB-2022-026

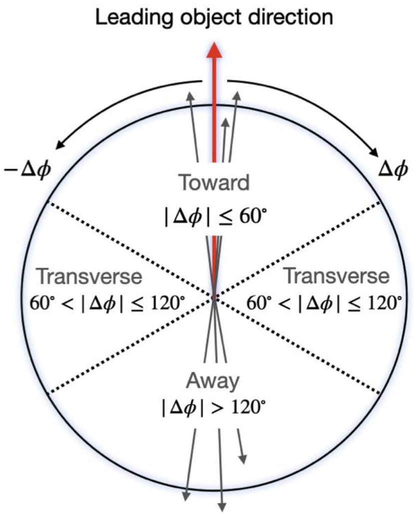
Table 4: The list of observables used for the comparison of the generators for the $t\bar{t}b\bar{b}$ process.

Variable	Description	Channel
$\Delta R_{bb}^{\min\Delta R}$	ΔR of the two b-jets in the event which are closest in ΔR	dilepton
$m_{bb}^{\min\Delta R}$	Invariant mass of the two b-jets closest in ΔR	dilepton
N_{jets}	Number of jets in the event (all jet flavours)	dilepton
Light jet p_{T}	Transverse momentum of the light jets in the event	dilepton
$N_{b\text{-jets}}$	Number of b-jets in the event	single lepton
$H_{\text{T}}^{\text{jets}}$	Scalar sum of p_{T} of jets in the event (all jet flavours)	single lepton
Leading b-jet p_{T}	p_{T} of b-jet with largest p_{T} in the event	single lepton
Fourth b-jet p_{T}	p_{T} of b-jet with fourth largest p_{T} in the event	single lepton

Pythia 8 color reconnection tunes based on UE data in CMS

CMS-GEN-17-002

- Different regions of the plane transverse to the direction of the beams are generally considered, as defined by the direction of the leading charged particle.
  - A **“toward” region** mainly includes the products of the hard scattering,
  - two **“transverse” regions** contain the products of MPI and are affected by contributions from ISR and FSR,
  - an **“away”** region comprises the recoiling objects belonging to the hard scattering.

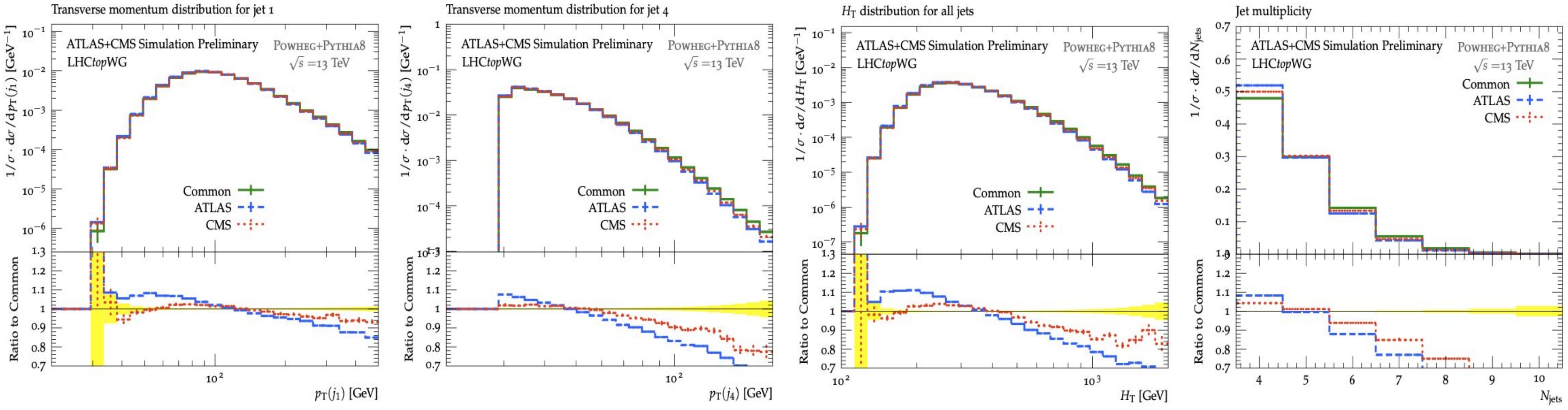


- The transverse region can be subdivided into a “transMIN” and a “transMAX”
  - regions with the minimum and maximum number of particles between the two transverse regions.
  - This is done in order to try to disentangle in a better way contributions from MPI, ISR, and FSR.
  - For events with large initial or final-state radiation the transMAX region contains the “transverse-side” jet, while both the transMAX and transMIN regions receive contributions from the MPI and beam-beam remnants.
  - **the transMIN region is sensitive to the MPI and BBR, while the transMAX minus the transMIN is very sensitive to initial and final-state radiation.**

Towards common $t\bar{t}$ MC settings for ATLAS and CMS

ATL-PHYS-PUB-2021-016, CMS-NOTE-2021-005

- Common settings vs ATLAS and CMS nominal settings

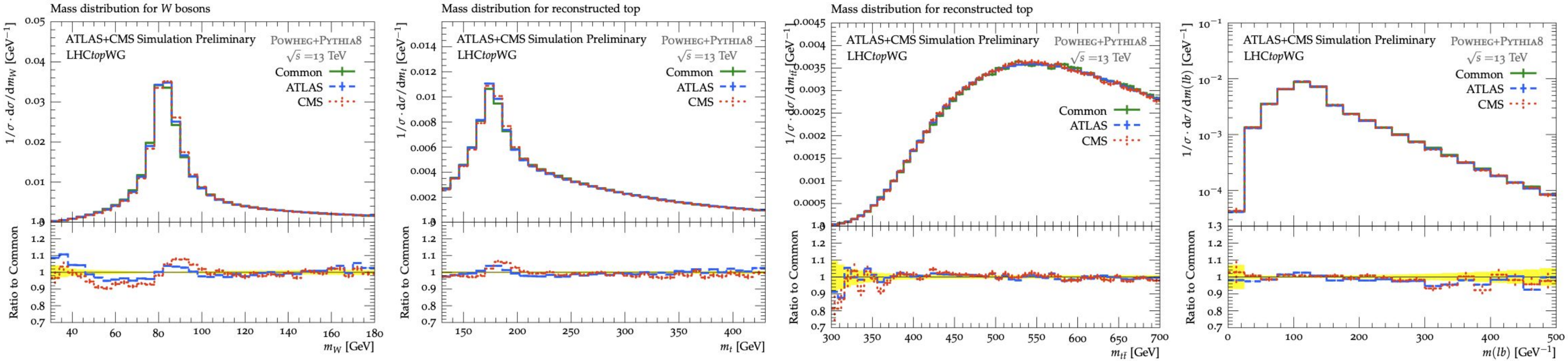


- Disagreement found in many distributions, particularly those related to jet kinematics and resonance masses
- The Monash tune and a harder value of α_s in the common sample lead to a harder p_T spectrum and more energy in the event

Towards common $t\bar{t}$ MC settings for ATLAS and CMS

ATL-PHYS-PUB-2021-016, CMS-NOTE-2021-005

- Common settings vs ATLAS and CMS nominal settings

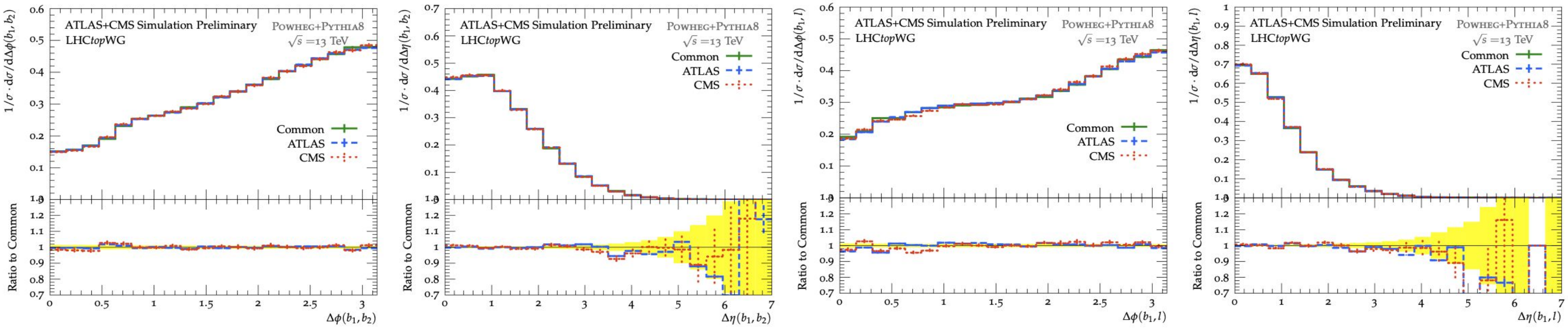


- Both the W mass and the top mass are shifted slightly in the peak of the distribution for the common sample compared to the other samples, even though the input masses are the same
  - ➪ Can be attributed to differences in parton shower model, the α_S value (which affects out-of-cone radiation) and the colour reconnection modelling
- Both the m_{tt} and m_{lb} distributions show overall good agreement between all samples, with some slight disagreement between the common sample and the nominal samples at low m_{tt} values

Towards common $t\bar{t}$ MC settings for ATLAS and CMS

ATL-PHYS-PUB-2021-016, CMS-NOTE-2021-005

- Common settings vs ATLAS and CMS nominal settings



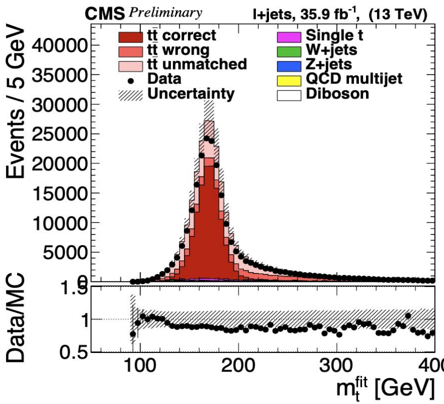
- Good agreement is observed between all three samples in angular distributions sensitive to spin correlation effects

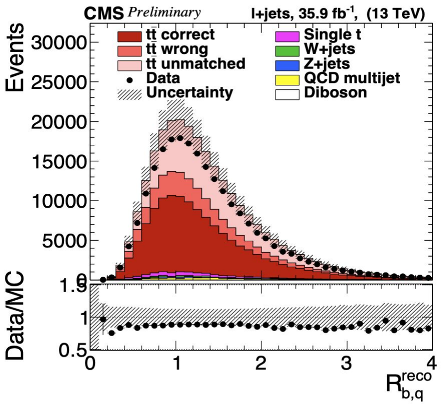
Profile likelihood approach to measure top quark mass in CMS

CMS-PAS-TOP-20-008

More details in M. Vanadia's talk

- Direct measurement of m_{top} in the l+jets channel
- First direct measurement using standard MC templates fit to 13 TeV data could not improve on results from CMS Run 1 legacy (PRD 93, 2016, 072004)
  - Uncertainties dominated by jet energy correction and color reconnection modelling
- New study includes:
  - Legacy data reconstruction
  - CP5 UE tune
  - MC samples with higher stats
  - Extended set of systematic variations
- New mass extraction method
  - Include all sources of uncertainty as nuisance parameters in the likelihood
  - Prior knowledge from templates derived on distributions that depend on m_{top} or can help constrain some systematics
  - Five independent observables are used:
    - Fit to m_{top}
    - Reconstructed mass W and lb system
    - $m_{reco,lb}/m_{fit,top}$, uncorrelated to $m_{fit,top}$ and less sensitive to jet energy
    - $R^{reco}_{bq} = \frac{p^{reco}_{T_{b1}} + p^{reco}_{T_{b2}}}{p^{reco}_{T_{q1}} + p^{reco}_{T_{q2}}}$, (used by ATLAS in EPJC-79-290), gives an additional handle on flavor-dependent jet energy scales.

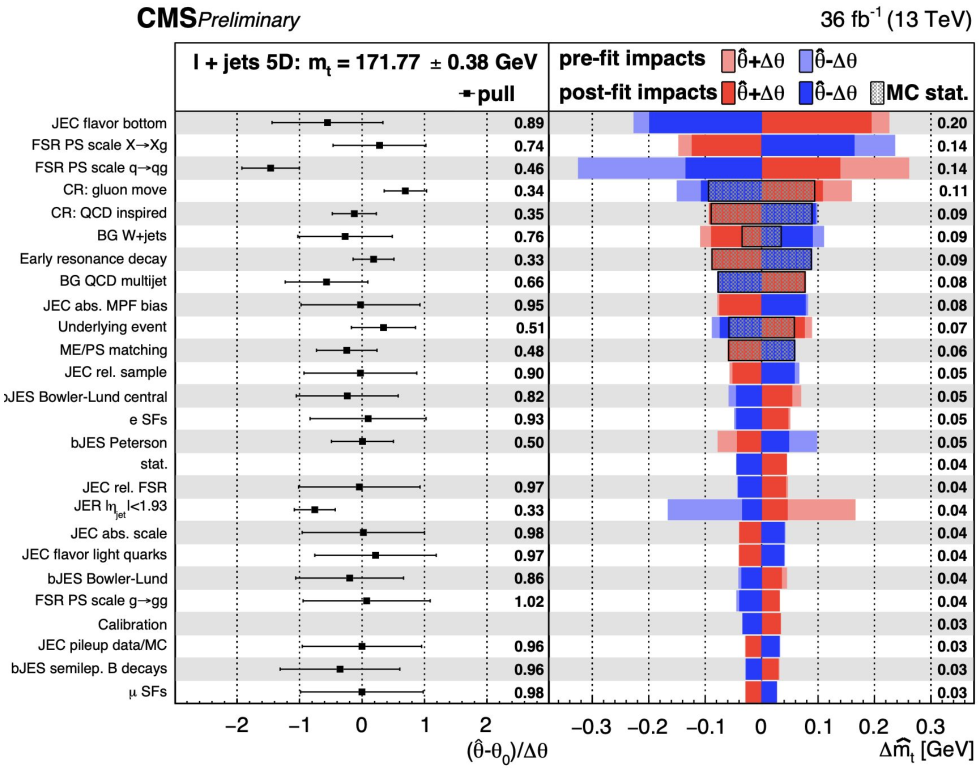




Profile likelihood approach to measure top quark mass in CMS

CMS-PAS-TOP-20-008

- Profile LH approach including more observables and nuisance parameters helps reduce systematic uncertainties



- The final result is 171.77 ± 0.38 GeV, including 0.04 GeV statistical uncertainty
- Measurement still dominated by jet energy correction and color reconnection
- JER strongly constrained in the fit
- Final State Radiation (FSR) Parton Shower (PS) scale uncertainties bigger than in previous analyses
- Impact of statistics of MC samples still considerable
- Most precise top quark mass measurement!